2-Methoxyethyl acetate

110-49-6 | DTXSID2025553

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.31 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.27e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

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Tetrahydrothiophene
Measured: 2.00
Predicted: 13.4

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bis(2-Chloro-1-methylethyl) ether
Measured: 3.92
Predicted: 1.62

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Acetal
Measured: 10.8
Predicted: 33.8

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Heptanoic acid
Measured: 2.34
Predicted: 6.20e-03

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8-Methylquinoline
Measured: 55.4
Predicted: 1.23e-02